An alternative construction of the positive inner product for pseudo-Hermitian Hamiltonians: Examples

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This paper builds on our earlier proposal for construction of a positive inner product for pseudo-Hermitian Hamiltonians and we give several examples to clarify our method. We show through the example of the harmonic oscillator how our construction applies equally well to Hermitian Hamiltonians which form a subset of pseudo-Hermitian systems. For finite dimensional pseudo-Hermitian matrix Hamiltonians we construct the positive inner product (in the case of 2×2 matrices for both real as well as complex eigenvalues). When the quantum mechanical system cannot be diagonalized exactly, our construction can be carried out perturbatively and we develop the general formalism for such a perturbative calculation systematically (for real eigenvalues). We illustrate how this general formalism works out in practice by calculating the inner product for a couple of $\mathcal{PT}$ symmetric quantum mechanical theories.

I. INTRODUCTION

In a recent paper [1] we described a systematic procedure for constructing the positive inner product for a quantum mechanical systems described by a pseudo-Hermitian Hamiltonian which satisfies [2]

$$H = S^{-1}H^\dagger S. \tag{1}$$

Here S is a bounded operator which can be chosen to be Hermitian (in the sense of Dirac). The crucial concept in our construction is the knowledge of the generators of energy eigenstates which acting on a given reference state generate all the eigenstates of the Hamiltonian. The method works equally well for systems with real or complex energy eigenvalues. We note that a pseudo-Hermitian Hamiltonian reduces to a Hermitian Hamiltonian when $S = \mathbb{1}$ and, therefore, our construction of the positive inner product also reduces to the standard Dirac inner product in this case (which we discuss in section **III**). In [1] we illustrated the method through the example of the Lee model [3, 4] with an imaginary coupling constant [5]. In this paper we give additional examples within the context of finite dimensional matrix Hamiltonians (which are pseudo-Hermitian) to clarify our method.

However, most quantum mechanical systems cannot be solved exactly. As a result, it is not possible to determine the energy eigenstates of the system and, therefore, their generators in a closed form. As we observed in [1], in such a case, the generator as well as the inner product can be determined only perturbatively. (The pseudo-Hermitian systems differ from the Hermitian systems in this respect, namely, the inner product of the system depends on the dynamics of the system in a nontrivial

manner [2, 6, 7, 8].) In this paper, we would like to develop the idea of a perturbative determination of the inner product in detail for real energy eigenvalues (the discussion for complex energy values is straightforward) and work out various $\mathcal{PT}$ symmetric [6, 7] examples to illustrate the method.

The paper is organized as follows. In section **II**, we briefly recapitulate our proposal for constructing the positive inner product in a pseudo-Hermitian quantum mechanical system, clarifying some of the details not fully explained in [1]. In section **III**, we apply our method to the case of the harmonic oscillator which can be taken as the unperturbed Hamiltonian in some of the examples we discuss. In section **IV**, we work out in detail a pseudo-Hermitian 2×2 matrix model with real and complex eigenvalues in an analogy with [9]. We also discuss the method in the context of $n \times n$ matrix models. In section **V** we describe the general formalism for the perturbative determination of the generator of energy eigenstates and, therefore, the perturbative construction of the positive inner product (for real energy values). In section **VI**, we apply the general method to various $\mathcal{PT}$ symmetric quantum mechanical models with real energy eigenvalues. We conclude with a brief summary in section **VII**.

II. RECAPITULATION OF THE CONSTRUCTION OF THE INNER PRODUCT

In this section, we briefly recapitulate the essential points discussed in [1] in the construction of the inner product in a pseudo-Hermitian quantum mechanical system described by (1). We showed that if we define an operator

$$q = SA, \tag{2}$$

where $[A, H] = 0$, and choose A properly, then the quadratic form

$$\langle \phi | \psi \rangle_q = \langle \phi | q | \psi \rangle, \qquad (3)$$

defines an inner product (on a suitably defined Hilbert space, see [1] for details) satisfying

$$\langle \psi_{E'} | \psi_E \rangle_q = \delta_{E\bar{E}'}, \qquad (4)$$

with a unitary time evolution. Here and in what follows a bar denotes complex conjugation. The operator q can be systematically constructed from a knowledge of the generators of the energy eigenstates of the theory in the following way.

An operator σ_E satisfying the relation

$$H\sigma_E = E\sigma_E + \sigma_E k_E, \qquad (5)$$

is defined to be a generator of the eigenstates of H with eigenvalue E provided

(i) there exists at least one vector $|\psi\rangle$, solving

$$k_E |\psi\rangle = 0, \quad \text{for all } E \in \text{spect}(H), \qquad (6)$$

with $\sigma_E |\psi\rangle \neq 0$.

(ii) there exists at least one vector $|\phi\rangle$ solving

$$k_E^\dagger |\phi\rangle = 0, \quad \text{for all } E \in \text{spect}(H), \qquad (7)$$

with $\langle \psi | \phi \rangle \neq 0$.

(iii) σ_E has an inverse σ_E^{-1}, at least acting on the reference state $|\psi\rangle$, such that

$$\sigma_E^{-1}\sigma_E |\psi\rangle = |\psi\rangle, \qquad (8)$$

and an adjoint inverse, $(\sigma_E^\dagger)^{-1}$, well-defined when acting on $|\phi\rangle$, with $(\sigma_E^\dagger)^{-1} |\phi\rangle \neq 0$.

From (5) and (6), it follows that

$$|\psi_E\rangle = \sigma_E |\psi\rangle, \qquad (9)$$

is an eigenvector of H with eigenvalue E. Similarly, from the (Dirac) adjoint of (5) as well as using (7), we can show that

$$|\phi_E\rangle = (\sigma_E^\dagger)^{-1} |\phi\rangle, \qquad (10)$$

is an eigenvector of $H^\dagger$ with eigenvalue $\bar{E}$. Furthermore, if P_E denotes projection operator on to the energy eigenstate $|\psi_E\rangle$ with energy E

$$P_E |\psi_{E'}\rangle = \delta_{EE'} |\psi_E\rangle, \qquad (11)$$

then we showed in [1] that the action of q can be expressed as

$$q(\sigma_E |\psi\rangle) = (\sigma_{\bar{E}}^\dagger)^{-1}|\phi\rangle. \qquad (12)$$

As a result q has the operator form

$$q = \sum_E (\sigma_{\bar{E}}^\dagger)^{-1} q_0 \sigma_E^{-1} P_E, \qquad (13)$$

where we have identified

$$|\phi\rangle = q_0 |\psi\rangle, \quad \text{such that} \quad \langle \psi | \phi \rangle = \langle \psi | q_0 | \psi \rangle = 1. \quad (14)$$

We note that in practical calculations, it is sufficient to have a partial inverse [*] σ_E^{-1} as we will demonstrate in the next section.

The construction (5)-(14) is quite general. It holds for pseudo-Hermitian Hamiltonians with real or complex eigenvalues. It also works for Hermitian Hamiltonians (which is a subset of pseudo-Hermitian Hamiltonians) for which $S = \mathbb{1}$ and in this case the operator q can be chosen to be $q = \mathbb{1}$ leading us back to the Dirac inner product. In [1] we applied this construction to calculate q for the Lee model [3, 4] with an imaginary coupling [5]. The purpose of the present paper is to work out more examples of diverse nature in order to shed more light on this method. It was pointed out in [1] that when the exact eigenstates of the Hamiltonian are not known, the generators as well as q can be constructed perturbatively and one of the goals of the present work is to describe systematically how such a perturbative calculation works. In the next section we apply our method to the case of the harmonic oscillator which can be taken as the zeroth order Hamiltonian in some of the subsequent examples where we determine q perturbatively. The Hamiltonian for the harmonic oscillator is, of course, Hermitian and this would also show how our method leads back to the standard Dirac inner product in cases where the Hamiltonian is Hermitian.

III. HARMONIC OSCILLATOR

Before we determine q for finite dimensional matrix models and discuss how q can be determined perturbatively in systems where the exact energy eigenstates are not known, let us describe how the construction of the last section works in the simple example of the harmonic oscillator. In this case, we expect the inner product to coincide with the standard Dirac inner product and, therefore, we expect to be able to show that we can choose $q = \mathbb{1}$.

The Hamiltonian for the harmonic oscillator can be written as

$$H_{\text{h.o.}} = \frac{1}{2}(p^2 + x^2 - 1) = a^\dagger a = H_{\text{h.o.}}^\dagger, \qquad (15)$$

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[*]A valid partial inverse can be found by noting that the generators are not unique. In fact, if σ_E is a generator for H then $\tilde{\sigma}_E = f(H)\sigma_E$ is also a generator (with the same reference state $|\psi\rangle$). For the harmonic oscillator we get that $(\sigma^{-1})^\dagger = 1/a$ as the generator for $H^\dagger$, but we prefer to use instead $H^\dagger(\sigma^{-1})^\dagger = a^\dagger$.

where $a, a^\dagger$ denote respectively the annihilation and the creation operators defined by

$$a = \frac{1}{\sqrt{2}}(x + ip), \quad a^\dagger = \frac{1}{\sqrt{2}}(x - ip), \qquad (16)$$

and we have subtracted out the zero point energy in (15) for simplicity. Here we have also set $m = \omega = 1 = \hbar$ for simplicity. The energy eigenstates of the oscillator are well known and satisfy

$$H_{\text{h.o.}}|\psi_{E_n}\rangle = E_n|\psi_{E_n}\rangle = n|\psi_n\rangle, \quad n = 0, 1, 2, \cdots. \quad (17)$$

Therefore, we can write the normalized eigenstates as

$$|\psi_{E_n}\rangle = |\psi_n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}|\psi_0\rangle, \quad a|\psi_0\rangle = 0, \qquad (18)$$

where $|\psi_0\rangle$ denotes the ground state of the system (commonly denoted by $|0\rangle$) and the energy eigenstates satisfy the orthonormality relation (with respect to the Dirac inner product)

$$\langle\psi_m|\psi_n\rangle = \delta_{mn}. \qquad (19)$$

We see from (18) that we can identify the reference state with the ground state and the generator of the energy eigenstates as

$$|\psi\rangle = |\psi_0\rangle, \quad \sigma_{E_n} = \sigma_n = \frac{(a^\dagger)^n}{\sqrt{n!}}. \qquad (20)$$

Furthermore, from the canonical commutation relation $[a, a^\dagger] = \mathbb{1}$, it follows that

$$H_{\text{h.o.}}\sigma_n = E_n\sigma_n + \sigma_n H_{\text{h.o.}}, \qquad (21)$$

where we have used $E_n = n$. Comparing this with (5) we determine that in the present case

$$k_{E_n} = k_n = H_{\text{h.o.}}, \qquad (22)$$

which indeed satisfies

$$k_n|\psi\rangle = H_{\text{h.o.}}|\psi_0\rangle = 0. \qquad (23)$$

It also follows that for the present problem

$$|\phi\rangle = |\psi\rangle = |\psi_0\rangle, \quad q_0 = \mathbb{1}. \qquad (24)$$

The partial inverse of the generator (8) can also be determined from the canonical commutation relation to be

$$\sigma_n^{-1} = \frac{a^n}{\sqrt{n!}}, \quad \sigma_n^{-1}\sigma_n|\psi\rangle = |\psi\rangle. \qquad (25)$$

We emphasize here that only a partial inverse is necessary for our construction which allows us to avoid awkward terms of the form $(a^\dagger)^{-n}$ for the inverse. We also note

that the projection operators for the energy eigenstates, in this case, can be written in the simple form

$$P_{E_n} = P_n = |\psi_n\rangle\langle\psi_n|, \quad \sum_n P_n = \mathbb{1}, \qquad (26)$$

which satisfies

$$\frac{(a^\dagger)^n}{\sqrt{n!}} \frac{a^n}{\sqrt{n!}} P_n = P_n. \qquad (27)$$

With all these, we can now determine q (see (13)) to be

$$\begin{aligned} q &= \sum_E (\sigma_{E_n}^{-1})^\dagger q_0 \sigma_{E_n}^{-1} P_{E_n} = \sum_n \frac{(a^\dagger)^n}{\sqrt{n!}} \frac{a^n}{\sqrt{n!}} P_n \\ &= \sum_n P_n = \mathbb{1}, \end{aligned} \qquad (28)$$

so that the inner product (3), in this case, coincides with the standard Dirac inner product

$$\langle\phi|\psi\rangle_q = \langle\phi|q|\psi\rangle = \langle\phi|\psi\rangle. \qquad (29)$$

It is worth emphasizing here that the relation (5) defining the generator does not determine its scale uniquely, namely, the generator is defined only up to a multiplicative factor. If we had defined the generators in (20) as $\sigma_n = c_n(a^\dagger)^n$ instead (giving $\sigma_n^{-1} = \frac{a^n}{c_n n!}$), (13) would lead to

$$q = \sum_n \frac{1}{|c_n|^2 n!} P_n. \qquad (30)$$

Thus, we see that we can choose any coefficient multiplying the generators and it will change q by a constant factor at each P_n. However, any choice of σ_n enforces $\langle\psi_n|\psi_n\rangle_q = 1$. In particular, this determines that $q = \mathbb{1}$ for $c_n = \frac{1}{\sqrt{n!}}$ reducing the inner product to the Dirac product.

IV. PSEUDO-HERMITIAN MATRIX HAMILTONIANS

In this section we discuss in detail two examples where we describe how our method applies to finite dimensional matrix Hamiltonians which are in general pseudo-Hermitian. The finite dimensional matrix Hamiltonians can be solved exactly in principle.

A. 2×2 matrix

As the first example, we apply our method to a simple 2×2 matrix Hamiltonian with real as well as complex eigenvalues. We recall that the $\mathcal{PT}$ symmetric 2×2 matrix model described by the Hamiltonian (see [9] for details)

$$H^{(\mathcal{PT})} = \begin{pmatrix} re^{i\theta} & s \\ s & re^{-i\theta} \end{pmatrix}, \qquad (31)$$

has been studied extensively in the past. Let us, therefore, analyze the generalized 2×2 matrix Hamiltonain (r, s, t, θ, ϕ are real parameters)

$$H = \begin{pmatrix} r\,e^{i\theta} & s\,e^{i\phi} \\ t\,e^{-i\phi} & r\,e^{-i\theta} \end{pmatrix}, \qquad (32)$$

which is not Hermitian unless $s = t, \theta = 0$. For $s = t, \phi = 0$ this model reduces to the $\mathcal{PT}$ symmetric theory (31) where the parity operation is identified with

$$\mathcal{P} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \mathcal{P}^\dagger, \quad \mathcal{P}^2 = \mathbb{1}, \qquad (33)$$

with $\mathcal{T}$ denoting complex conjugation. The Hamiltonian in (32), however, is not $\mathcal{PT}$ symmetric in this context. On the other hand, if we define a "generalized parity" operation through the 2×2 matrix

$$\widetilde{\mathcal{P}} = \begin{pmatrix} 0 & \sqrt{\frac{s}{t}} \\ \sqrt{\frac{t}{s}} & 0 \end{pmatrix}, \qquad (34)$$

and choose time reversal to correspond to complex conjugation, then it is easily verified that the general Hamiltonian (32) is $\widetilde{\mathcal{PT}}$ symmetric, namely,

$$\widetilde{\mathcal{PT}} H \widetilde{\mathcal{PT}} = H. \qquad (35)$$

The "generalized parity" operator in (34) reduces to (33) when $s = t$. In general, however, let us note that while this operator is idempotent, it is not Hermitian,

$$\widetilde{\mathcal{P}}^2 = \mathbb{1}, \quad \widetilde{\mathcal{P}}^\dagger \neq \widetilde{\mathcal{P}}. \qquad (36)$$

Furthermore, unlike the case in $\mathcal{PT}$ symmetric theories [6, 7] (where $\mathcal{P} H \mathcal{P} = H^\dagger$ and, therefore $\mathcal{P}$ defines the matrix S in (1)), here we have

$$\widetilde{\mathcal{P}} H \widetilde{\mathcal{P}} = H^* \neq H^\dagger. \qquad (37)$$

Therefore, $\widetilde{\mathcal{P}}$ cannot be identified with S in (1) which is used in our construction. However, we can define an operator (2×2 matrix)

$$S = \begin{pmatrix} 0 & e^{i\phi} \\ e^{-i\phi} & 0 \end{pmatrix} = S^\dagger = S^{-1}, \qquad (38)$$

which leads to

$$H = S^{-1} H^\dagger S. \qquad (39)$$

In other words, even though $\widetilde{P}$ does not take the Hamiltonian to its Hermitian conjugate, S does and the general Hamiltonian H in (32) is pseudo-Hermitian and our method can be directly applied.

The energy eigenvalues of this system are given by

$$E_\pm = r\,\cos\theta \pm \sqrt{st - r^2 \sin^2\theta}, \qquad (40)$$

and they are real for $st > r^2 \sin^2\theta$ while they are complex for $st < r^2 \sin^2\theta$. (We do not consider the degenerate case $st = r^2 \sin^2\theta$, for which the Hamiltonian cannot be diagonalized, simply because it would introduce pseudo-eigenvectors.) We would analyze the two cases separately in the following.

1. Real eigenvalues:

In the case of real eigenvalues, let us define

$$Q = \sqrt{st - r^2 \sin^2\theta} = \text{real}, \qquad (41)$$

so that the two real energy eigenvalues can be written as

$$E_\pm = r\,\cos\theta \pm Q = \bar{E}_\pm. \qquad (42)$$

The corresponding eigenvalues can be determined to have the forms

$$|\psi_{E_+}\rangle = \frac{1}{\sqrt{s+t}} \begin{pmatrix} \left(\frac{s}{t}\right)^{1/4} \sqrt{Q + ir\,\sin\theta}\, e^{i\phi/2} \\ \left(\frac{t}{s}\right)^{1/4} \sqrt{Q - ir\,\sin\theta}\, e^{-i\phi/2} \end{pmatrix},$$

$$|\psi_{E_-}\rangle = \frac{i}{\sqrt{s+t}} \begin{pmatrix} \left(\frac{s}{t}\right)^{1/4} \sqrt{Q - ir\,\sin\theta}\, e^{i\phi/2} \\ -\left(\frac{t}{s}\right)^{1/4} \sqrt{Q + ir\,\sin\theta}\, e^{-i\phi/2} \end{pmatrix}, (43)$$

which have been normalized in the conventional sense for simplicity (although it is not necessary). We note that the two energy eigenstates are also eigenstates of $\widetilde{\mathcal{PT}}$ with eigenvalue 1 (they correspond to singlet states under $\widetilde{\mathcal{PT}}$), namely,

$$\widetilde{\mathcal{PT}}|\psi_{E_+}\rangle = |\psi_{E_+}\rangle, \quad \widetilde{\mathcal{PT}}|\psi_{E_-}\rangle = |\psi_{E_-}\rangle. \qquad (44)$$

The projection operators onto the two states are given by

$$P_{E_+} = \frac{1}{2Q} \begin{pmatrix} Q + ir\,\sin\theta & s\,e^{i\phi} \\ t\,e^{-i\phi} & Q - ir\,\sin\theta \end{pmatrix},$$

$$P_{E_-} = \frac{1}{2Q} \begin{pmatrix} Q - ir\,\sin\theta & -s\,e^{i\phi} \\ -t\,e^{-i\phi} & Q + ir\,\sin\theta \end{pmatrix}. \qquad (45)$$

Let us choose the reference state (see (6) or (9))

$$|\psi\rangle = |\psi_{E_-}\rangle. \qquad (46)$$

It follows now from (43) that the generators of the states are given by

$$\sigma_{E_+} = \begin{pmatrix} 0 & i\sqrt{\frac{s}{t}}\,e^{i\phi} \\ -i\sqrt{\frac{t}{s}}\,e^{-i\phi} & 0 \end{pmatrix} = \sigma_{E_+}^{-1},$$

$$\sigma_{E_-} = \mathbb{1}, \quad k_{E_-} = -k_{E_+} = 2Q P_{E_+}. \qquad (47)$$

The reference state (7) can also be determined to be

$$|\phi\rangle = -\left(\frac{s+t}{2Q}\right) S|\psi\rangle = q_0|\psi\rangle, \quad q_0 = -\left(\frac{s+t}{2Q}\right) S, \qquad (48)$$

where the reference state has been normalized according to (14). It follows now from (13) (using (47) as well as (48)) that

$$q = \sigma_{E_+}^\dagger q_0 \sigma_{E_+} P_{E_+} + \sigma_{E_-} q_0 \sigma_{E_-} P_{E_-}$$

$$= \left(\frac{s+t}{2Q}\right) S \left(P_{E_+} - P_{E_-}\right)$$

$$= \frac{s+t}{2Q^2} \begin{pmatrix} t & -ir\,\sin\theta\, e^{i\phi} \\ ir\,\sin\theta\, e^{-i\phi} & s \end{pmatrix}. \qquad (49)$$

It can be checked now that

$$\langle\psi_{E_i}|q|\psi_{E_j}\rangle = \langle\psi_{E_i}|\psi_{E_j}\rangle_q = \delta_{ij}, \quad i, j = \pm. \qquad (50)$$

2. Complex eigenvalues:

For the case $st < r^2 \sin^2 \theta$, as we have noted the eigenvalues are complex and let us define

$$\widetilde{Q} = \sqrt{r^2 \sin^2 \theta - st} = \text{real}, \tag{51}$$

so that the two energy eigenvalues (40) which become complex conjugate pairs can be written as

$$E = r \cos \theta - i\widetilde{Q}, \quad \bar{E} = r \cos \theta + i\widetilde{Q}. \tag{52}$$

The two eigenstates can be determined to have the forms

$$\begin{aligned}
|\psi_E\rangle &= \frac{(-i)}{\sqrt{(s+t)r \sin \theta + (s-t)\widetilde{Q}}} \\
&\quad \times \begin{pmatrix} i\sqrt{s(r \sin \theta - \widetilde{Q})}\, e^{i\phi/2} \\ \sqrt{t(r \sin \theta + \widetilde{Q})}\, e^{-i\phi/2} \end{pmatrix}, \\
|\psi_{\bar{E}}\rangle &= \frac{i}{\sqrt{(s+t)r \sin \theta + (s-t)\widetilde{Q}}} \\
&\quad \times \begin{pmatrix} \sqrt{s(r \sin \theta + \widetilde{Q})}\, e^{i\phi/2} \\ -i\sqrt{t(r \sin \theta - \widetilde{Q})}\, e^{-i\phi/2} \end{pmatrix}, \tag{53}
\end{aligned}$$

It s clear that the eigenstates (53) of the Hamiltonian for complex eigenvalues correspond to a doublet representation of $\widetilde{\mathcal{PT}}$ (compare with (44)), namely,

$$\widetilde{\mathcal{PT}}|\psi_E\rangle = |\psi_{\bar{E}}\rangle, \quad \widetilde{\mathcal{PT}}|\psi_{\bar{E}}\rangle = |\psi_E\rangle. \tag{54}$$

The projection operators onto these two states take the forms

$$\begin{aligned}
P_E &= \frac{1}{2\widetilde{Q}} \begin{pmatrix} -(r \sin \theta - \widetilde{Q}) & is\, e^{i\phi} \\ it\, e^{-i\phi} & r \sin \theta + \widetilde{Q} \end{pmatrix}, \\
P_{\bar{E}} &= \frac{1}{2\widetilde{Q}} \begin{pmatrix} r \sin \theta + \widetilde{Q} & -is\, e^{i\phi} \\ -it\, e^{-i\phi} & -(r \sin \theta - \widetilde{Q}) \end{pmatrix}. \tag{55}
\end{aligned}$$

Let us next choose the reference state

$$|\psi\rangle = |\psi_E\rangle. \tag{56}$$

It follows now from (53) that the generators of states are given by

$$\begin{aligned}
\sigma_{\bar{E}} &= \begin{pmatrix} 0 & -\sqrt{\frac{s}{t}}\, e^{i\phi} \\ \sqrt{\frac{t}{s}}\, e^{-i\phi} & 0 \end{pmatrix} = -\sigma_{\bar{E}}^{-1}, \\
\sigma_E &= \mathbb{1}, \quad k_E = -k_{\bar{E}} = 2i\widetilde{Q}P_{\bar{E}}. \tag{57}
\end{aligned}$$

The reference state (7) can now be obtained to have the form

$$|\phi\rangle = q_0 |\psi\rangle = -\frac{(s+t)r \sin \theta + (s-t)\widetilde{Q}}{2\sqrt{st}\,\widetilde{Q}} \sigma_{\bar{E}}^\dagger S |\psi\rangle, \tag{58}$$

where

$$q_0 = -\frac{(s+t)r \sin \theta + (s-t)\widetilde{Q}}{2\sqrt{st}\,\widetilde{Q}} \begin{pmatrix} \sqrt{\frac{t}{s}} & 0 \\ 0 & -\sqrt{\frac{s}{t}} \end{pmatrix}. \tag{59}$$

It can be checked that this state satisfies

$$k_E^\dagger |\phi\rangle = k_{\bar{E}}^\dagger |\phi\rangle = 0, \quad \langle \psi | \phi \rangle = \langle \psi | q_0 | \psi \rangle = 1. \tag{60}$$

It follows now from (13) (using (57) as well as (59)) that

$$\begin{aligned}
q &= -\sigma_{\bar{E}}^\dagger q_0 P_E - q_0 \sigma_{\bar{E}} P_{\bar{E}} \\
&= -\frac{(s+t)r \sin \theta + (s-t)\widetilde{Q}}{2\sqrt{st}\,\widetilde{Q}} S(P_E + P_{\bar{E}}) \\
&= -\frac{(s+t)r \sin \theta + (s-t)\widetilde{Q}}{2\sqrt{st}\,\widetilde{Q}} S. \tag{61}
\end{aligned}$$

It is easy to check that

$$\langle \psi_E | \psi_E \rangle_q = 0 = \langle \psi_{\bar{E}} | \psi_{\bar{E}} \rangle_q, \quad \langle \psi_{\bar{E}} | \psi_E \rangle_q = 1. \tag{62}$$

In this case, we note that the operator q simply scales the operator S in (38) which leads to the pseudo-Hermitian nature of the Hamiltonian.

B. n × n matrix

Here we will solve for the operator q for an n-dimensional Hilbert space, so that q will be an $n \times n$ matrix. We will assume that the Hamiltonian H has n real, distinct eigenvalues (no degeneracies) so that H has a diagonal Jordan decomposition. Therefore, we can find an invertible matrix R such that

$$R^{-1}HR = H_0, \tag{63}$$

where $H_0 = \text{diag}\{E_1, E_2, ..., E_n\}$. Because H_0 is diagonal there exists a basis of vectors, $|v_i\rangle$ satisfying,

$$H_0 |v_i\rangle = E_i |v_i\rangle, \quad \langle v_j | v_i \rangle = \delta_{ji}, \quad E_i = \bar{E}_i, \tag{64}$$

for $1 \le i, j \le n$.

However, in the non-diagonal basis, the eigenstates for H are given by $|\psi_i\rangle = R|v_i\rangle$. The Dirac-inner product of two such states is

$$\langle \psi_i | \psi_j \rangle = \langle v_i | R^\dagger R | v_j \rangle, \tag{65}$$

and is generally not orthonormal with respect to the eigenstates $|\psi_i\rangle$. We can modify the inner product by introducing an operator q as discussed in the previous section,

$$\langle \psi_i | \psi_j \rangle_q = \langle \psi_i | q | \psi_j \rangle = \delta_{ij}. \tag{66}$$

In order to restore orthonormality it would appear from (65) and (66) that we should choose $q = (R^{-1})^\dagger R^{-1}$. On the other hand, we recall from (13) that

$$q = \sum_{i=1}^n (\sigma_{E_i}^{-1})^\dagger q_0 \sigma_{E_i}^{-1} P_i, \tag{67}$$

where $\sigma_{E_i}|\psi\rangle = |\psi_i\rangle$ defines the generators of states, $P_j|\psi_i\rangle = \delta_{ij}|\psi_i\rangle$ defines the projection operators, and q_0 is the matrix satisfying $q_0|\psi\rangle = |\phi\rangle$, $\langle\psi|\phi\rangle = 1$, for the reference states $|\psi\rangle$, $|\phi\rangle$.

To show that the two definitions are in fact equivalent, let us choose the reference state to be $|\psi\rangle = |\psi_n\rangle$. Since $|\psi_n\rangle = R|v_n\rangle$, this implies that $|\phi\rangle = (R^{-1})^\dagger|v_n\rangle$ (because we want $\langle\phi|\psi\rangle = 1$ to hold). Furthermore, since $q_0|\psi_n\rangle = q_0|\psi\rangle = |\phi\rangle$, then using $P_n = R|v_n\rangle\langle v_n|R^{-1} = |\psi_n\rangle\langle\psi_n|q$ we can write the identity

$$q_0 P_n = q P_n. \tag{68}$$

(We note that although q_0 is generally different from q, it must act the same way on the reference state $|\psi_n\rangle$.)

Second, we observe that in the diagonal basis, $|v_i\rangle$, there exists an upper-triangular matrix t satisfying $t|v_i\rangle = |v_{i+1}\rangle$, with $t|v_n\rangle = |v_1\rangle$, and $t^\dagger = t^{-1}$ (t is just the matrix with ones above the diagonal, and one in the lower left-hand corner). This gives $\sigma_{E_i} = \sigma^i = Rt^iR^{-1}$ (here t^i denotes the i th power of t), where $\sigma = RtR^{-1}$ defines the generator of states. The statement $\sigma^{-i}P_i = P_n\sigma^{-i}$ is evident.

Using our definitions above, we can calculate directly

$$
\begin{aligned}
q &= \sum_{i=1}^n (\sigma^{-i})^\dagger q_0 \sigma^{-i} P_i \\
&= \sum_{i=1}^n (\sigma^{-i})^\dagger q_0 P_n \sigma^{-i} = \sum_{i=1}^n (\sigma^{-i})^\dagger q P_n \sigma^{-i} \\
&= \sum_{i=1}^n ((R^{-1})^\dagger t^i R^\dagger)((R^{-1})^\dagger R^{-1}) P_n (Rt^{-i}R^{-1}) \\
&= (R^{-1})^\dagger \left(\sum_{i=1}^n |v_i\rangle\langle v_i| \right) R^{-1} \\
&= (R^{-1})^\dagger R^{-1}. \tag{69}
\end{aligned}
$$

In finite dimensional Hilbert spaces, such as this, it is probably easier to calculate $q = (R^{-1})^\dagger R^{-1}$ directly from the Jordan matrices R (which consist of each eigenvector of H in one of the columns). However, in infinite dimensional Hilbert spaces there is no Jordan decomposition, but the operators σ_E which generate the eigenvectors do exist. Thus, our expression for q is valid in both finite, and infinite dimensions, whether or not one can construct the Jordan matrix. As we will see in the next two sections, there exist operators (also denoted by R) which will play a role very similar to the Jordan matrix given above. These will turn out to be the perturbation operators.

V. PERTURBATIVE DETERMINATION OF q

Let us next consider a pseudo-Hermitian system with real energy eigenvalues (as in $\mathcal{PT}$ symmetric theories [6, 7]) where the energy eigenstates may be difficult to

determine exactly. In this case, let us assume that we can write the pseudo-Hermitian Hamiltonian H as

$$H = H_0 + \epsilon V(x), \tag{70}$$

where H_0 is the part of the Hamiltonian H which we can diagonalize and we treat $\epsilon V(x)$ as a perturbation. Of course, H_0 can be Hermitian or non-Hermitian. However, in most practical examples, it can be chosen to be Hermitian and this is the case we will discuss here. Let us denote the generators for the eigenstates of H_0 by $\sigma_E^{(0)}$ so that we can express the eigenstates of H_0 as

$$|\psi_E^{(0)}\rangle = \sigma_E^{(0)}|\psi\rangle, \tag{71}$$

where $|\psi\rangle$ denotes the reference state for the system (see (6) and (9)). Since H_0 is chosen to be Hermitian, as in the case of the harmonic oscillator, it follows that (see (24))

$$|\psi\rangle = |\phi\rangle, \quad q_0 = \mathbb{1}. \tag{72}$$

Thus, for the (diagonalizable) unperturbed part of the Hamiltonian we can determine (see (28))

$$
\begin{aligned}
q^{(0)} &= \sum_E (\sigma_E^{(0)\,-1})^\dagger \, q_0 (\sigma_E^{(0)})^{-1} \, P_E^{(0)} \\
&= \sum_E (\sigma_E^{(0)\,-1})^\dagger \, (\sigma_E^{(0)})^{-1} \, P_E^{(0)} = \mathbb{1}, \tag{73}
\end{aligned}
$$

as we have seen in (28). Here $P_E^{(0)} = |\psi_E^{(0)}\rangle\langle\psi_E^{(0)}|$ is the projection onto an eigenstate of H_0 with eigenvalue $E^{(0)}$.

The eigenstates of the total Hamiltonian H in (70) can be written as a series in powers of the perturbation parameter ϵ, namely, (ϵ^i denotes the ith power of ϵ)

$$|\psi_E\rangle = \sum_i \epsilon^i|\psi_E^{(i)}\rangle, \tag{74}$$

where $|\psi_E^{(i)}\rangle$ denotes the ith order correction to the state $|\psi_E^{(0)}\rangle$. We can always choose the corrections to a given state to be orthogonal to the state, namely,

$$\langle\psi_E^{(0)}|\psi_E^{(i)}\rangle = 0, \quad i > 0. \tag{75}$$

In this case, the perturbative corrections to the state $|\psi_E^{(0)}\rangle$ can be obtained to have the compact recursive form ($i > 0$ and we are assuming the energy eigenvalues to be discrete)

$$
\begin{aligned}
|\psi_E^{(i)}\rangle &= \sum_{E'\neq E} \frac{1}{E^{(0)} - E'^{(0)}} \times \\
&\left(\langle\psi_{E'}^{(0)}|V|\psi_E^{(i-1)}\rangle - \sum_{j=1}^{i-1} E^{(j)} \langle\psi_{E'}^{(0)}|\psi_E^{(i-j)}\rangle \right) |\psi_{E'}^{(0)}\rangle \\
&= R^{(i)}|\psi_E^{(0)}\rangle = R^{(i)}\sigma_E^{(0)}|\psi\rangle = \sigma_E^{(i)}|\psi\rangle, \tag{76}
\end{aligned}
$$

where $R^{(i)}$ denotes the operator that transforms the unperturbed state $|\psi_E^{(0)}\rangle$ to $|\psi_E^{(i)}\rangle$ and

$$E^{(i)} = \langle \psi_E^{(0)}|V|\psi_E^{(i-1)}\rangle, \quad i > 0. \qquad (77)$$

From (76) we note that we can define the correction to the generator of the state at the ith order as

$$\sigma_E^{(i)} = R^{(i)}\sigma_E^{(0)}, \qquad (78)$$

with the same (zeroth order) reference state $|\psi\rangle$. Therefore, to any order in perturbation we can write

$$
\begin{aligned}
R &= \sum_{i=0} \epsilon^i R^{(i)}, \\
\sigma_E &= \sum_{i=0} \epsilon^i \sigma_E^{(i)} = \sum_{i=0} \epsilon^i R^{(i)}\sigma_E^{(0)} = R\sigma_E^{(0)}, \quad (79)
\end{aligned}
$$

where $R^{(0)} = \mathbb{1}$. By taking the adjoint of (70), and using $|\phi\rangle = |\psi\rangle$ (see (72)), we likewise determine the corrections to the eigenstates of $H^\dagger$ to any order to be (see (10))

$$|\phi_E\rangle = (R^{-1})^\dagger|\phi_E^{(0)}\rangle = (R^{-1})^\dagger(\sigma_E^{(0)\,-1})^\dagger\,|\psi\rangle, \qquad (80)$$

with the same reference state $|\psi\rangle$.

Puting this into the equation for q (see (13)) we find that for real E (recall that we are considering a pseudo-Hermitian system with real energy eigenvalues as in $\mathcal{PT}$ symmetric theories)

$$
\begin{aligned}
q &= \sum_E (\sigma_E^{-1})^\dagger\, \sigma_E^{-1}\, P_E \\
&= (R^{-1})^\dagger \left(\sum_E (\sigma_E^{(0)\,-1})^\dagger\, \sigma_E^{(0)\,-1}\, P_E^{(0)} \right) R^{-1} \\
&= (R^{-1})^\dagger\, q^{(0)}\, R^{-1}, \qquad (81)
\end{aligned}
$$

where $q^{(0)}$ is the q operator for the unperturbed Hamiltonian which, for a Hermitian H_0, is given by $q^{(0)} = \mathbb{1}$ (see (73)). In this case, therefore, (81) reduces to

$$q = (R^{-1})^\dagger R^{-1}. \qquad (82)$$

For real eigenvalues, we see that q only depends on the perturbation operator R, and that the problem is solved once we determine R from perturbation theory. If we had not chosen H_0 to be Hermitian, then $q^{(0)}$ in (81) would be nontrivial which would need to be determined as well.

VI. EXAMPLES

In this section we would work out two examples of $\mathcal{PT}$ symmetric theories (with real energy eigenvalues) to illustrate how the perturbative calculation is carried out in practice. We recall from (82) that when the unperturbed Hamiltonian H_0 is Hermitian, then to any order in the perturbing parameter, the operator q is determined from the operator R defined in (78)- (79) to that order.

A. Example: $H = \frac{1}{2}(p^2 + x^2 - 1) + i\epsilon x^3$

Let us consider the Hamiltonian given by [10],

$$H = \frac{1}{2}(p^2 + x^2 - 1) + i\epsilon x^3 = H_0 + \epsilon V(x), \qquad (83)$$

where ϵ is a real constant parameter and we recognize that $H_0 = H_{\text{h.o.}}$ describes the harmonic oscillator which we have studied in section **III** (we continue to identify $m = \omega = 1 = \hbar$). This model is known to be $\mathcal{PT}$ symmetric with real energy eigenvalues and has been studied extensively in the past. Here we would calculate the operator q (which defines the inner product) associated with this system perturbatively using our method.

The Hamiltonian for the harmonic oscillator is Hermitian and the system can be solved exactly. As a result, we can choose $H_0 = H_{\text{h.o.}}$ to be the unperturbed Hamiltonian in which case we can take over the analysis of section **V**. We have already seen in (18) and (20) that the generator for the harmonic oscillator has a very simple form. Therefore, for the unperturbed system we can identify

$$|\psi_n^{(0)}\rangle = \sigma_n^{(0)}|\psi_0\rangle = \sigma_n^{(0)}|\psi\rangle, \quad E_n^{(0)} = n. \qquad (84)$$

Furthermore, recalling that $x = \frac{1}{\sqrt{2}}(a + a^\dagger)$ (see, (16)), the first order correction to the unperturbed eigenstate can be determined from (76) as

$$
\begin{aligned}
|\psi_n^{(1)}\rangle &= \sum_{m \neq n} \frac{\langle \psi_m|ix^3|\psi_n\rangle}{E_n^{(0)} - E_m^{(0)}}|\psi_m\rangle \\
&= \frac{i}{2^{3/2}}\Big(\frac{1}{3}a^3 + 3\{a^2 a^\dagger\} - 3\{a^{\dagger 2}a\} - \frac{1}{3}a^{\dagger 3}\Big)|\psi_n\rangle \\
&= \frac{i}{2^{3/2}}\Big(-\frac{2}{3}(a - a^\dagger)^3 + \{(a + a^\dagger)^2(a - a^\dagger)\}\Big) \\
&= -\Big(\frac{2}{3}p^3 + x^2 p - ix\Big)|\psi_n^{(0)}\rangle \\
&= -\Big(\frac{2}{3}p^3 + x^2 p - ix\Big)\sigma_n^{(0)}|\psi\rangle. \qquad (85)
\end{aligned}
$$

Thus, comparing with (79) we determine that to first order in perturbation

$$R = R^{(0)} + \epsilon R^{(1)} = \mathbb{1} - \epsilon\Big(\frac{2}{3}p^3 + x^2 p - ix\Big). \qquad (86)$$

Similarly, carrying out the perturbative calculation to order ϵ^3 we determine (see (79))

$$R = \mathbb{1} + \epsilon R^{(1)} + \epsilon^2 R^{(2)} + \epsilon^3 R^{(3)}, \qquad (87)$$

where

$$R^{(1)} = -\left(\frac{2}{3}p^3 + x^2p - ix\right),$$

$$R^{(2)} = \left(\frac{23}{288}p^6 + \frac{23}{96}x^2p^4 - \frac{i}{48}xp^3 + \frac{7}{96}x^4p^2 \right.$$
$$\left. -\frac{1}{16}p^2 + \frac{13i}{48}x^3p + \frac{11}{8}x^2 - \frac{41}{288}x^6\right),$$

$$R^{(3)} = \left(\frac{59}{1296}p^9 + \frac{59}{288}x^2p^7 - \frac{593i}{288}xp^6 - \frac{163}{120}p^5 \right.$$
$$+\frac{109}{288}x^4p^5 - \frac{1591i}{288}x^3p^4 - \frac{769}{48}x^2p^3$$
$$+\frac{307}{864}x^6p^3 + \frac{649i}{48}xp^2 - \frac{443i}{96}x^5p^2$$
$$-\frac{17}{12}p - 13\,x^4p + \frac{41}{288}x^8p$$
$$\left. +\frac{685i}{72}x^3 - \frac{287i}{288}x^7\right). \quad (88)$$

To this order, therefore, we can calculate

$$R^{-1} = \mathbb{1} - \epsilon R^{(1)} - \epsilon^2\left(R^{(2)} - (R^{(1)})^2\right)$$
$$-\epsilon^3\left(R^{(3)} + (R^{(1)})^3 - R^{(1)}R^{(2)} - R^{(2)}R^{(1)}\right). (89)$$

And from this we can calculate q to order ϵ^3 (see (82)) to have the manifestly Hermitian form,

$$q = \mathbb{1} - \epsilon\left(\frac{4}{3}p^3 + 2xpx\right) + \epsilon^2\left(\frac{169}{144}p^6 + \frac{169}{48}xp^4x\right.$$
$$+\frac{137}{48}px^4p + \frac{41}{144}x^6 - \frac{177}{8}x^2\right)$$
$$+\epsilon^3\left(-\frac{181}{3}p - \frac{41}{36}x^4px^4 + \frac{457}{24}x^2px^2\right.$$
$$-\frac{523}{108}x^3p^3x^3 + \frac{3463}{60}p^5 + \frac{5669}{72}xp^3x$$
$$\left. -\frac{253}{36}x^2p^5x^2 - \frac{155}{36}xp^7x - \frac{155}{162}p^9\right) + O(\epsilon^4). \quad (90)$$

This can be compared with [10] to find linear order agreement. The difference in higher order terms is due to our choice of normalization $\langle\psi|\psi\rangle_q = \langle\psi|q|\psi\rangle = 1$.

It is worth noting here that in this case the perturbing Hamiltonian is parity odd while the free harmonic oscillator Hamiltonian is invariant under parity (each term is individually $\mathcal{PT}$ invariant). As a result, the zeroth order energy eigenstates $|\psi_n^{(0)}\rangle$ are parity eigenstates and at every even order $|\psi_n^{(i)}\rangle$ would have the same parity as $|\psi_n^{(0)}\rangle$ while at every odd order $|\psi_n^{(i)}\rangle$ would have the opposite parity. This leads to the fact that at odd order (where the correction to the energy can become imaginary)

$$E_n^{(i)} = 0, \quad i = 2m+1. \quad (91)$$

The even order corrections to energy, on the other hand, are all real. Therefore,

$$E_n = \sum_{i=0} \epsilon^{2i} E_n^{(2i)}, \quad (92)$$

is real at any order of perturbation. This is an alternative way of understanding the reality of energy in this model.

B. Example: $H = \frac{1}{2}(p^2 + x^2 - 1) + i\alpha x + i\epsilon x^3$

From the previous results it is a simple matter to calculate q in the case of the $\mathcal{PT}$ symmetric theory described by

$$H = \frac{1}{2}(p^2 + x^2 - 1) + i\alpha x + i\epsilon x^3, \quad (93)$$

where α, ϵ are real constant parameters. First we note that with the canonical commutation relations we can write (see (15))

$$e^{-\alpha p/2}\,H_{\text{h.o.}}\,e^{\alpha p/2} = H_{\text{h.o.}} + i\alpha x - \alpha^2/4. \quad (94)$$

Therefore, in this case, we can write (93)

$$H = e^{-\alpha p/2}\,H_{\text{h.o.}}\,e^{\alpha p/2} + \alpha^2/4 + i\epsilon x^3 = H_0 + i\epsilon x^3, \quad (95)$$

where we have identified

$$H_0 = e^{-\alpha p/2}\,H_{\text{h.o.}}\,e^{\alpha p/2} + \alpha^2/4. \quad (96)$$

We can take this H_0 to be the free Hamiltonian in this case for which

$$E_n^{(0)} = E_n^{(\text{h.o.})} + \alpha^2/4, \quad |\psi_n^{(0)}\rangle = e^{-\alpha p/2}|\psi_n^{(\text{h.o.})}\rangle. \quad (97)$$

We can now carry over the perturbative analysis of the previous example on this state and determine q (and, therefore, the inner product) to any order from

$$q = ((Re^{-\alpha p/2})^{-1})^\dagger (Re^{-\alpha p/2})^{-1} = (R^{-1})^\dagger\,e^{\alpha p}\,R^{-1}, (98)$$

with R calculated in the previous example.

These two examples illustrate how the perturbative determination works when the exact energy eigenstates are difficult to obtain.

VII. SUMMARY

In this paper we have tried to build on our earlier proposal [1] for determining the positive inner product in the case of a pseudo-Hermitian Hamiltonian. The crucial concept in our method is the generator of energy eigenstates. We have clarified various aspects of our proposal which were not possible to explain in the earlier paper. We have shown through the example of the harmonic oscillator how our proposal reduces to the standard Dirac inner product when the Hamiltonian is Hermitian. We have given (additional) examples of finite dimensional pseudo-Hermitian matrix Hamiltonians to explain how our method works in practice. When the quantum mechanical Hamiltonian cannot be diagonalized exactly, the generator as well as the inner product need to be constructed perturbatively. We have developed the general

formalism for this systematically for real energy eigenvalues. Furthermore, we have applied the formalism to two $\mathcal{PT}$ symmetric Hamiltonians to illustrate how it is carried out in practice.

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